Scope of Work For

Project #22-023
Source-Sector NOx Emissions Analysis with sub-kilometer Scale Airborne Observations in Houston during TRACER-AQ

Prepared for

Air Quality Research Program (AQRP)
The University of Texas at Austin

By

Daniel Goldberg (Principal Investigator)
George Washington University
Washington, D.C.

Jeremiah Johnson (Co-Principal Investigator)
Greg Yarwood
Ramboll
Novato, CA

August 16, 2022
Version #1

QA Requirements: Audits of Data Quality: 10% Required
Report of QA Findings: Required in Final Report

NOTE: The workplan package consists of three independent documents: Scope of Work, Quality Assurance Project Plan (QAPP), and budget and justification.

Approvals

This Scope of Work was approved electronically on **08/23/2022** by Elena McDonald-Buller, The University of Texas at Austin

Elena McDonald-Buller
Project Manager, Texas Air Quality Research Program

This Scope of Work was approved electronically on **9/12/2022** by Madison Knapp, Texas Commission on Environmental Quality

Madison Knapp
Project Liaison, Texas Commission on Environmental Quality

Table of Contents

1.0 Abstract

Nitrogen oxide (NO_X) emissions are a critical participant in ozone formation. Many North American cities already have NO_X-limited ozone formation during the warm season (Jin et al., 2020; Jung et al., 2022), and the remaining cities should have primarily NO_X-limited conditions in the coming years (Koplitz et al., 2021). Further reducing ozone production rates within cities will therefore require improved quantification of NO_X emissions. One major limitation of our current observing network is the inability to accurately quantify NO_X emissions on a sector-by-sector basis in a timely fashion, with the exception of continuous emissions monitoring systems (CEMS) on electricity generating units. Many non-road sources of NO_X emissions, such as industrial or construction emissions, have large uncertainties (Zawacki et al., 2018).

In this project we will use fine spatial resolution nitrogen dioxide (NO_2) information (250 × 560 m^2) from the Geostationary Coastal and air pollution events Airborne Simulator (GCAS) instrument (Janz et al., 2019; Nowlan et al., 2018), available during the September 2021 NASA/TCEQ Tracking Aerosol Convection ExpeRiment – Air Quality (TRACER-AQ) field campaign, to better understand the fine-scale structure of NO_X emissions in the Houston metropolitan area including a sector-by-sector analysis.

Complementing the airborne observations, the Comprehensive Air Quality Model with Extensions (CAMx) will be run with a fine spatial resolution (444 × 444 m^2) using the 2019 TCEQ emissions inventory. The model output will then be compared to data from the GCAS and the Tropospheric Monitoring Instrument (TROPOMI) in order to identify gaps in our understanding of NO_X emissions. We will compare/contrast NO_2 concentrations near large CEMS and non-CEMS point sources, major highways, large population centers, airports, railyards, and commercial marine vessels to determine whether the magnitude of the NO_X emissions agree between the inventory and observations. We will also use GCAS observations to estimate NO_X emissions directly from individual point sources or quasi-points sources (e.g., airports, petrochemical complexes, etc.). To maximize the value of the airborne measurements, we will use a Generalized Additive Model (GAM) to estimate the contributions from different NO_X emission sectors that best matches the airborne retrievals.

This work maps to at least four Research Priority Areas of the Texas Air Quality Research Program (AQRP), as shown in the table below. This project will combine aircraft and satellite observations with high resolution models, to provide actionable information about TCEQ's 2019 Emissions Inventory for NO_X. These results will provide a new perspective for aiding in decision-making for improving ozone air quality in the region.

Table 1. How this project will respond to the AQRP Research Priority Areas

Research Priority Area	How this project will be addressing the Research Priority
Utilize TRACER-AQ and over-water measurements	A central dataset used will be the GCAS measurements acquired during TRACER-AQ to infer sectorized NO_X emissions addressing TRACERAQ science objectives on Ozone Photochemistry and Model Evaluation

Improve emissions inventories	Satellite and aircraft measurements, aided by machine learning, will be used to directly estimate instantaneous NO_X emission rates, often from individual sources or sectors of sources such as on-road, non-road, commercial marine, and rail.
Improve accuracy of photochemical grid models	Model (CAMx) will be tested against the GCAS observations to identify where improvement is needed in NO_X emissions by sector, therefore improving model performance.
Use of satellite and other remote sensing data	Utilize aircraft (GCAS) and satellite (TROPOMI and TEMPO) to better understand spatial patterns of NO_2 and its relationship to NO_X emissions

2.0 Background

While fossil fuel consumption is known on a national basis with a high-degree of certainty, the spatial and temporal patterns of its combustion have a lesser degree of certainty (McDonald et al., 2013, 2012). The location and timing of the combustion emissions can substantially affect air quality; emissions in a rural area are not the same as emissions in an urban area due to the ambient environmental conditions and the higher probability of human exposure in urban settings.

Typically, air pollutant emission rates for chemical species such as nitrogen oxides (NOX) are estimated using a “bottom-up” approach, which uses fuel consumption information, spatial surrogates (e.g., road density, population density, locations of known stack emissions), temporal surrogates (e.g., traffic patterns, industrial work schedules) and emission factors (mass of pollutant per mass of fuel burned) to estimate the spatiotemporal patterns of emissions across regions. With investments in technology to better understand the spatiotemporal patterns of pollutants (e.g. incorporating real-time traffic data using speed and type of vehicle) and laboratory studies to better estimate the emission factors in a wide range of conditions, these “bottom-up” estimates can be improved. These new and improved estimates can then be incorporated into a chemical transport model and evaluated against observations from a ground monitoring network acquiring concentrations. Based on this comparison, the emission estimates can be further adjusted and improved if necessary. However, because of the complexity of this cycle, “bottom-up” emission estimates typically take many years to compile by a large team of scientists, and subsequently, are delayed in time by several years from the actual emission time.

A complementary approach to estimate air pollutant emissions is in using a “top-down” approach. With this method, emissions are back-calculated from pollutant measurements acquired across an entire airshed. This is typically done with a remote sensing instrument – in orbit (Goldberg et al., 2019b) or on an aircraft (Kuhlmann et al., 2022; Meier et al., 2017; Souri et al., 2018). The emission rates are inferred by analyzing the concentration maps over a large region and incorporating the lifetime (chemical and dispersion lifetime) of the pollutant to back-calculate the emission rate at the source. The advantage of this technique is that it is completely independent of the complex datasets needed to estimate “bottom-up” emissions rates. Further, while setting the foundation to do a “top-down” emission analysis can take some time (months/years), once the foundation is in-place, it is feasible that near-real-time emission rates could be derived within hours of the remote sensing measurement (Goldberg et al., 2019b).

Prior work by scientists on this team, sponsored by AQRP (Holloway et al., 2021), demonstrated the capability to estimate NOX emissions for the Dallas – Fort Worth metropolitan region for the summer of 2019 using a “top-down” approach and the Tropospheric Monitoring Instrument (TROPOMI). The team has also conducted similar analyses for other North American cities (Goldberg et al., 2019a, 2019b), power plants (de Foy et al., 2015), South Asia (de Foy and Schauer, 2022), and global megacities (Goldberg et al., 2021) using TROPOMI and a complementary satellite instrument, the Ozone Monitoring Instrument (OMI). The team is also already funded to estimate near-real-time NOX emissions using TROPOMI for several North American cities as part of a NASA Health and Air Quality Science Team (HAQAST) project grant. “Top-down” emission estimates can be helpful, especially in areas with very uncertain emission inventories such as Africa or the Middle East. Typically these aggregated “top-down” estimates agree with the “bottom-up” estimates within 20% in North American cities (well within the uncertainty associated with the ‘top-down’ method) (Goldberg et al., 2021). However, due to TROPOMI’s spatial resolution (3.5 × 5.5 km2 at nadir) and temporal resolution (once daily), TROPOMI is most often used to calculate total emissions aggregated over the entire metropolitan area. Therefore, very limited, if any, sector-by-sector resolved information can be gleaned from an analysis using currently available satellite datasets.

3.0 Objectives & Broader Implications

The overall objective of this work is to better understand the sector-by-sector NO_X emissions in the Houston metropolitan area using a combination of chemical transport models, aircraft observations, ground measurements, and satellite datasets. The broader implications of this study are to achieve a better understanding of the spatial and temporal patterns of ozone precursor emissions. Lessons learned and techniques developed for this project could be applied to other areas within Texas and potentially other areas in the United States. The project will also demonstrate the capability to: 1) estimate NO_X emissions using the GCAS and 2) quantify sectorized NO_X emissions from certain sources (non-CEMS point sources, airports, railyards, and commercial marine) that are difficult to constrain using typical "bottom-up" methodologies.

4.0 Task Descriptions

4.1 Task 1: Simulate NO2, HCHO, O3 at 444 × 444 m^2 spatial resolution using WRF-CAMx

We will run the Weather Research and Forecasting (WRF) model and the Comprehensive Air Quality Model with Extensions (CAMx) at 444 × 444 m^2 spatial resolution for the Houston metropolitan area for September 2021 using emission inventory data from the TCEQ. CAMx will be run with source apportionment of NO_2 to track contributions from up to 10 emission sectors, including EGUs, on-road mobile, shipping and rail. Meteorological conditions will be simulated using WRF to drive the CAMx 444 × 444 m^2 grid. These grid resolutions nest within an existing 4 km grid with meshing ratios of 3 and 9. Ramboll will perform the model simulations and is experienced working with these models and the TCEQ's emission data.

Model simulations will be conducted by enhancing an existing high-resolution WRF-CAMx model platform for 2019 developed for TCEQ (Near Real-Time Exceptional Event Model; NRTEEM) described in Johnson et al. (2018) and Holloway et al. (2021). WRF and CAMx modeling domains at 36, 12, and 4 km are used for the NRTEEM system. The 36 km domain includes all of the continental US and large areas of Central America and Canada; the 12 and 4 km domains are TCEQ State Implementation Plan (SIP) domains, which are used for other modeling efforts by the TCEQ and Ramboll. Chemical analysis is performed by CAMx v7.20 with input meteorology calculated by WRF version 4.4 with GFS 0.25° × 0.25° analysis data for initial/boundary conditions.

We will define the 444 m^2 CAMx grid to include the most relevant Houston TRACER-AQ flight path segments. This domain will be nested within an outer 1.33 km^2 CAMx grid that uses boundary conditions from a separate 36/12/4 km CAMx simulation using the domains described above.

We will use anthropogenic emissions from the 2019 TCEQ modeling inventory (closest to 2021 available) and September 2021 hourly CEMS data for power plants. We will refine the spatial resolution of line-source emission sectors (i.e., roads, rail, and marine shipping) to the 444 m^2 grid. TCEQ will provide link-based emissions for both on-road and rail emissions. We will use the MARINe Emissions Reslover (MARINER) tool to generate commercial marine vessel (CMV) emissions at 444 m resolution from Automatic Identification System (AIS) ship identification and tracking information. Point sources provided by TCEQ will also be resolved to 444 m. Biogenic emissions will be calculated using the Model of Emissions of Gases and Aerosols from Nature (MEGAN) version 3.1 developed by Ramboll in AQRP project 18-005 (Guenther et al., 2012).

The modeling team will create grids of source-apportioned NO_2 concentrations as well as HCHO, and O_3 between the surface and the top of the troposphere. Two different column amounts will be calculated from this information: the vertical column between the surface and ~9 km (to match the GCAS observations) and the vertical column between the surface and ~13 km (to match the satellite observations), although the difference between these two vertical extents will be well within the uncertainty of satellite, GCAS, and modeling datasets.

Once preliminary results from model/aircraft/satellite intercomparison are available (Tasks 5 & 6), the model will be re-run to test the effectiveness of the adjustments to the NO_X emissions.

4.2 Task 2: Process the GCAS measurements

GCAS NO_2 column measurements were acquired during NASA G-V flights on 10 different days over the Houston metropolitan area during September 2021 as part of the NASA / TCEQ TRACER-AQ field campaign (https://www-air.larc.nasa.gov/missions/tracer-aq/docs/TRACERAQ_SciencePlan_v1.pdf). All GCAS data are publicly available at the NASA Langley data archive: https://www-air.larc.nasa.gov/cgi-bin/ArcView/traceraq.2021.

Figure 1 shows late afternoon NO_2 from September 8, 2021, a code red ozone day in the Houston metropolitan area demonstrating the granularity of information provided.

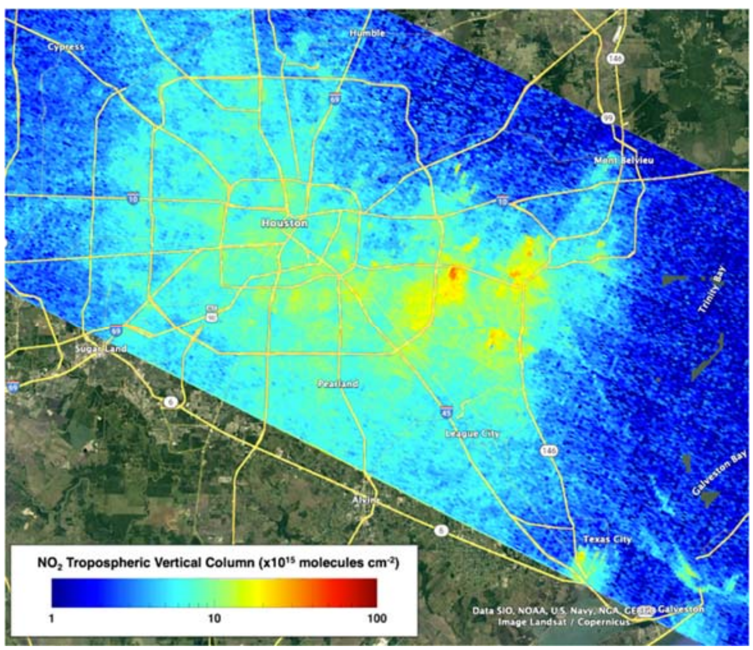

Figure 1. NO_2 vertical column amounts between the surface and 28,000 ft acquired from the GCAS approximately between 2:20 PM CT and 5 PM CT on Sept 8, 2021.

GCAS measures backscattered spectra in UV-Visible spectrum from an aircraft altitude of ~28,000 ft. Observed spectra in the 425-460 nm wavelength region are used to retrieve slant NO_2 column amounts by comparing the observed spectrum to a reference spectrum derived from observations over an unpolluted area (offset corrected by coincident TROPOMI observations) via Differential Optical Absorption

Spectroscopy (DOAS; (Platt and Stutz, 2008)). Next, the slant columns are converted into a vertical column densities using an air mass factor, which is primarily a function of surface reflectivities impacting the vertical sensitivity of the instrument and an a priori estimate of the NO_2 vertical profile shape factor (Palmer et al., 2001). Current GCAS vertical column NO_2 shape factors have been calculated using model information from the NASA GEOS Composition Forecast (GEOS-CF) replay (Keller et al., 2021). Versions of this retrieval from other studies have been well validated with the highly precise measurements from Pandora spectrometers with no systematic bias (Judd et al., 2020, 2019).

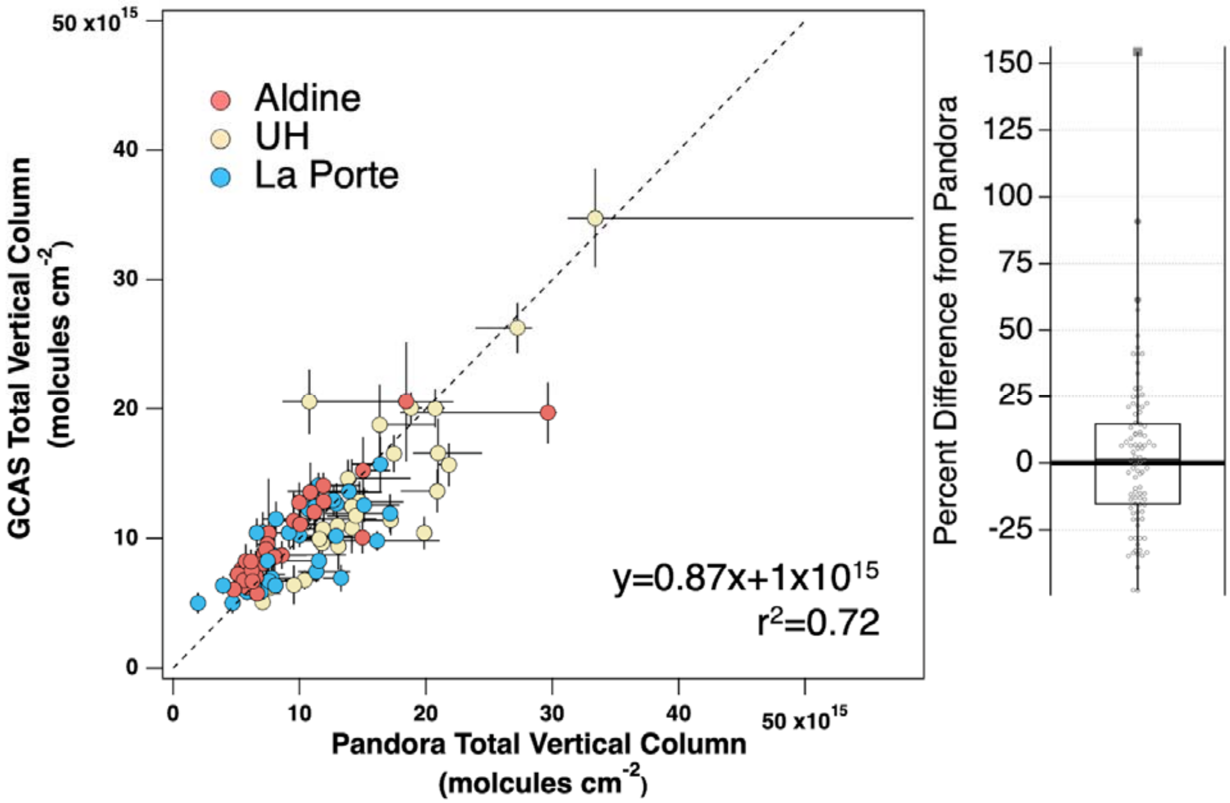

Figure 2. Comparison of the NO_2 total vertical column amounts between GCAS and the Pandora spectrometers during TRACER-AQ. Error bars represent the interquartiles of GCAS within 750 m of the Pandora and interquartiles of Pandora within 15 minutes of the GCAS overpass.

GCAS was first deployed in Houston during the DISCOVER-AQ Texas study in September 2013 (Nowlan et al., 2018), with precedent of using the high-resolution NO_2 observations to constrain NOx emissions within WRF-CMAQ (Souri et al., 2017). This proposed work takes it a step further by providing actionable information about sectorized emissions, rather than broader estimates on the emissions inventory as a whole. TRACER-AQ GCAS data is also less data sparse than the 2013 flights through the systematic gapless mapping conducted over the wider city of Houston (e.g., Figure 2), which was a noted weakness by Souri et al. (2017).

One advantage of the GCAS data is that it is available for different times of day, typically three times per day (early morning, late morning, and early afternoon). Visualizing the diurnal patterns of NO_2 by using the GCAS and Pandora measurements may help us elucidate some of the diurnal patterns of emissions.

For this project, we will work with Dr. Judd to further process the GCAS data. GCAS data will be re-gridded onto the 444 × 444 m^2 CAMx grid; this can be done even before the CAMx simulation is performed. Second, we will re-calculate the GCAS NO_2 vertical columns using the simulated NO_2 shape factor from the CAMx simulation to eliminate model dependencies on the results. Dr. Judd already has the software framework to re-calculate the GCAS vertical columns. These reprocessed GCAS NO_2 column data will be validated by directly comparing to the NO_2 column measurements from Pandora spectrometers at four stationary and two mobile sites during TRACER-AQ using methodology from Judd et al. (2020). Preliminary comparison of Pandora and GCAS for the publicly available dataset at 3 sites during TRACER-AQ (Aldine, University of Houston, and La Porte) shows good agreement with a median percent difference of 1.4% and an interquartile range of -15.5-14.9%.

4.3 Task 3: Process the satellite NO2 data

Measurements of tropospheric vertical column NO_2 from TROPOMI are available daily at approximately 1:45 PM local time during September 2021. We will screen the TROPOMI data for clouds and erroneous data using the recommended qa_flag > 0.75 filter. All TROPOMI NO_2 data are publicly available at: https://s5phub.copernicus.eu/dhus/#/home. Our group already has downloaded and filtered the data over Texas for May 2018 – April 2022, inclusive of September 2021 (Figure 3).

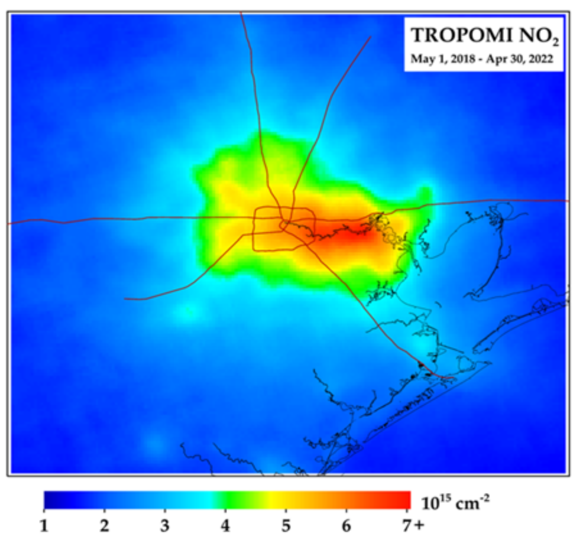

Figure 3. NO_2 tropospheric vertical column amounts acquired from the early PM overpasses of TROPOMI between May 2018 and Apr 2022.

For this task, we will re-grid the NO_2 column information onto the 444 × 444 m^2 CAMx grid, and re-calculate the NO_2 vertical columns using the simulated NO_2 column information from the CAMx simulation. Once re-gridded to the finer CAMx grid (444 × 444 m^2), the data can be averaged over the full month to get TROPOMI NO_2 averages at 444 × 444 m^2 spatial resolution. As part of AQRP project 20-020, software was developed to re-grid TROPOMI data to the CAMx model grid.

4.4 Task 4: Evaluate mobile emissions assessments performed with and without model

NO_X emission rates can be inferred from NO_2 using a combination of spatially continuous NO_2 airshed measurements, wind data, and statistical inversion techniques. By tracking the NO_2 plume decay since origination, the NO_X emissions at the source can be back-calculated. Two methods allow us to do this: 1) Exponentially modified Gaussian (EMG) fit (Beirle et al., 2011) and 2) Flux divergence (Beirle et al., 2019).

As part of AQRP project 20-020 (Goldberg et al., 2022; Holloway et al., 2021), we used both of these techniques to estimate NO_X emissions from the Dallas Fort Worth area using TROPOMI NO_2 data. For this project, we will more closely examine the Houston metropolitan area using both approaches on the satellite data and GCAS data where applicable. The major advances will come from the application of these methods on the GCAS data.

The EMG method does not work well when applied to current satellite observations (TROPOMI) over the Houston area due to the spatial asymmetry of emissions originating from the metropolitan area. However, we hypothesize that the increased spatial resolution of GCAS will allow us to derive NO_X emissions from some of the point and quasi-point sources in the metropolitan area. These will include the George Bush Intercontinental Airport (IAH), Mont Belvieu, Texas City, Baytown, and Deer Park. On individual days, the GCAS is observing individual well-defined NO_2 plumes originating from these areas (Figure 4).

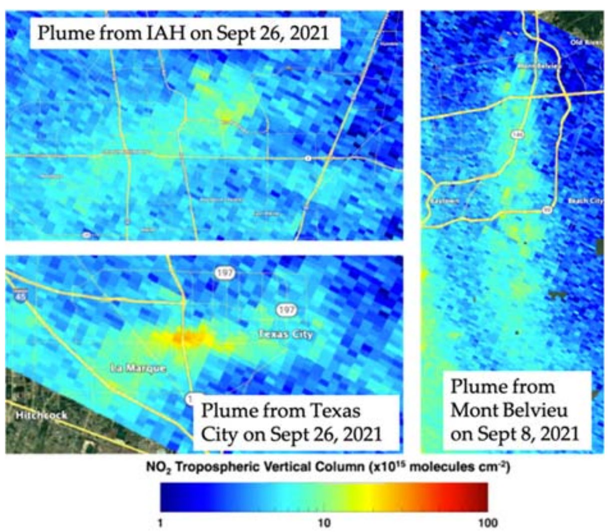

Figure 4. NO_2 plumes of quasi-point sources within the Houston metropolitan area acquired from GCAS.

The flux divergence method has been applied to the Houston area using TROPOMI data as a preliminary test. Whereas the total vertical columns of NO_2 show a fairly smooth dome of NO_2 above Houston (e.g., Figure 3), the flux divergence method was able to highlight known point sources and also show the importance of the ship channel as a main source of NOx. Furthermore, the flux divergence method was able to identify a corridor of higher NOx emission s extending from the city center to IAH. Given that the GCAS has a resolution that is more than 10 times finer than TROPOMI, we expect that analyzing flux divergences will provide even more detail at the level of individual sources. The method will be refined to handle the smaller number of scenes (27 maps collected over 10 days) as well as the different swath structure of the GCAS measurements so as to maximize the detection of specific emissions.

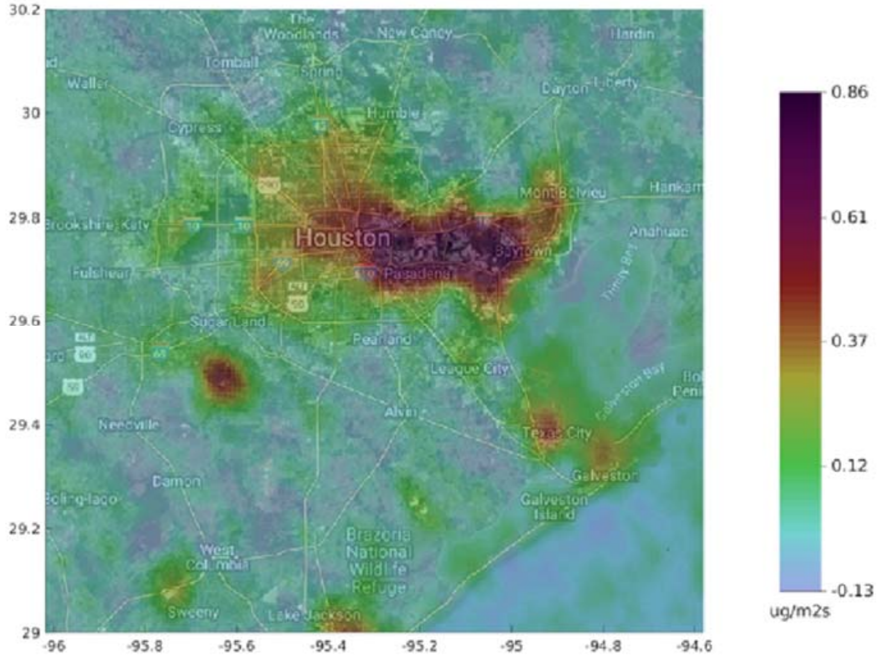

Figure 5. NO_2 Flux Divergence over Houston using TROPOMI NO_2 from Oct 2019 – Sept 2021 and ERA5 winds.

4.5 Task 5: Comparison of NO2, HCHO, O3 between model, aircraft, and satellite

Once the aircraft observations, satellite observations, and model simulation are all on the same model grid, then an intercomparison between the three datasets can be performed. As a prerequisite to this, we will need to process the GCAS (Task 2) and satellite (Task 3) observations using the NO_2 vertical profile information from CAMx. Without this step, aircraft, and satellite observations would be subject to artifacts related to their original a priori assumptions. After this is completed, it is appropriate to directly compare NO_2 from all three platforms to each other.

The analysis will compare NO_2 on a neighborhood scale (by zip code) and on a day-to-day basis when the three datasets (model, aircraft, and satellite) are collocated in time and space. A challenge of this comparison will be in controlling for dispersion/meteorological differences between the model and observations. Performing the model/GCAS comparison at a degraded spatial resolution ((i.e., zip code level) may resolve some of these dispersion-related differences.

In an additional analysis, we will rigorously compare NO_2 between the model and GCAS at several locations of the Houston metropolitan area known to have large NO_X emissions. These locations will include: downtown Houston, along the West Loop, IAH, Mont Belvieu, Texas City, Baytown, and Deer Park. Our team is open to feedback from AQRP on the selection of areas to investigate.

Under the scope of this task, we will also perform a comparison between the model and ground measurements for O_3. We will also perform a qualitative comparison between the modeled column HCHO, GCAS column HCHO, and TROPOMI column HCHO. Due the lower signal-to-noise ratio of the TROPOMI HCHO retrieval, we do not anticipate that the satellite observations of HCHO on a day-to-day basis will be particularly useful for this intercomparison.

4.5 Task 6: Use of machine learning to estimate emission factors for individual sectors

In parallel to Task 5, we will build a General Additive Model (GAM) (e.g., de Foy et al., 2021) to find the optimal combination of the sectoral emissions simulated by CAMx that matches the GCAS measurements. In order to maximize the information content of the GCAS instrument, we will do this in measurement space. The GAM seeks to reconstruct the measurements as a function of the sectoral NO_2 grids while also considering the impacts of possible confounding factors. Local meteorology, boundary layer heights, and land use patterns will be included in the model. The model will produce adjustment factors for NO_X emissions from each sector, which will be used to develop an optimized emission inventory (Figure 6). A second set of CAMx simulations will be conducted to test the level of improvement obtained by the procedure. The GAM method has been used extensively to obtain emission factors from time series measurements, but this would be a novel application enabled by the high resolution of the GCAS measurements. Finally, TCEQ will provide Harris County point source emissions inventory data for 2019 and 2021. We will compare these two inventories on a site level, source-sector level, and county level basis to determine differences in the estimated emissions. We will qualitatively compare these differences to the corrections made to the NOx source sectors in this task to evaluate if some of the corrections needed are due to a differences in the emissions inventories.

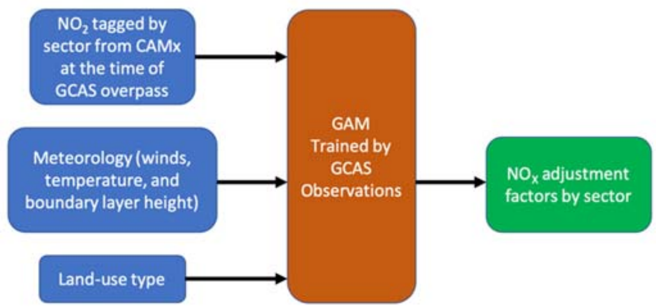

Figure 6. Workflow of the General Additive Model (GAM)

4.5 Task 7: Project Reporting and Presentations

As required, we will provide regular and timely submission of monthly technical reports, monthly financial status reports, and quarterly reports as well as an abstract at project initiation and, near the end of the project, submission of the draft final and final reports, according to the schedule outline in the Timeline. Dr. Goldberg, or a designee, will electronically submit each required report to both the AQRP and TCEQ liaisons and will follow the State of Texas accessibility requirements as set forth by the Texas State Department of Information Resources per http://aqrp.ceer.utexas.edu/. All drafts of planned presentations (such as at technical conferences), or manuscripts to be submitted for publication resulting from this project, will be provided to both the AQRP and TCEQ liaisons per the Publication/Publicity Guidelines. Data from the project at its completion will be submitted to the AQRP archive, including 444 × 444 m^2 gridded NO_2 data from GCAS, CAMx, and TROPOMI over the study domain and period. We plan to publish study results in a peer-reviewed scientific journal.

5.0 Project Participants and Responsibilities

Dr. Daniel Goldberg will lead the project as Principal Investigator, coordinate collaboration with Ramboll, and supervise the George Washington University research team. Dr. Greg Yarwood will serve as coPrincipal Investigator and lead the Ramboll modeling team. Dr. Laura Judd will be a Subject Matter Expert for the Team. Dr. Benjamin de Foy will be a co-I and consultant to George Washington University.

Dr. Greg Yarwood will oversee the emissions processing, and WRF-CAMx simulations. Dr. Daniel Goldberg and Dr. Laura Judd will process the GCAS data, satellite data, and ground measurement data. Dr. Daniel Goldberg and Dr. Benjamin de Foy will calculate the NO_X emissions from the GCAS data and satellite data using top-down techniques. A post-doctoral scientist at George Washington University will perform the GCAS and model intercomparison. A Masters student at George Washington University will organize group teleconferences and the monthly/quarterly/annual reports.

6.0 Timeline

During Aug 22, 2022 – Aug 31, 2023, the project will follow the timeline listed below:

Task	Name	S	O	N	D	J	F	M	A	M	J	J	A
1	Emissions preparation	X	X	X									
1	WRF Simulation	X	X	X									
1	CAMx simulation			X	X	X					X		
2	GCAS data preparation	X					X						
2	Compare GCAS to ground measurements	X	X	X	X	X							
3	TROPOMI data preparation & analysis	X	X				X						
3	TEMPO data preparation & analysis									X	X	X	
4	Estimating NOx emissions from GCAS directly	X	X	X	X								
5	Compare/contrast model to GCAS and satellite					X	X	X	X	X	X	X	
6	Use of machine learning map the impact of model sectoral emissions onto measurement space					X	X	X	X	X	X	X	
7	Monthly reports	X	X	X	X	X	X	X	X	X	X	X	
7	Financial reports	X	X	X	X	X	X	X	X	X	X	X	
7	Quarterly reports		X			X			X		X		
7	Annual report											X	X

7.0 Deliverables

AQRP requires certain reports to be submitted on a timely basis and at regular intervals. A description of the specific reports to be submitted and their due dates are outlined below. One report per project will be submitted (collaborators will not submit separate reports), with the exception of the Financial Status Reports (FSRs). The lead PI will submit the reports, unless that responsibility is otherwise delegated with the approval of the Project Manager. All reports will be written in third person and will follow the State of Texas accessibility requirements as set forth by the Texas State Department of Information Resources. Report templates and accessibility guidelines found on the AQRP website at http://aqrp.ceer.utexas.edu/ will be followed.

Abstract: At the beginning of the project, an Abstract will be submitted to the Project Manager for use on the AQRP website. The Abstract will provide a brief description of the planned project activities, and will be written for a non-technical audience.

Abstract Due Date: Tuesday, August 16, 2022

Quarterly Reports: The Quarterly Report will provide a summary of the project status for each reporting period. It will be submitted to the Project Manager as a Word doc file. It will not exceed 3 pages and will be text only. No cover page is required. This document will be inserted into an AQRP compiled report to the TCEQ.

Quarterly Report Due Dates:

Report	Period Covered	Due Date
Quarterly Report #1	August, September, October 2022	Monday, October 31, 2022
Quarterly Report #2	November, December 2022, January 2023	Tuesday, January 31, 2023
Quarterly Report #3	February, March, April 2023	Sunday, April 30, 2023
Quarterly Report #4	May, June, July 2023	Monday, July 31, 2023

Monthly Technical Reports (MTRs): Technical Reports will be submitted monthly to the Project Manager and TCEQ Liaison in Microsoft Word format using the AQRP FY22-23 MTR Template found on the AQRP website.

MTR Due Dates:

Report	Period Covered	Due Date
Technical Report #1	Project Start – August 31, 2022	Saturday, September 10, 2022

Technical Report #2	September 1 – 30, 2022	Monday, October 10, 2022
Technical Report #3	October 1 - 31, 2022	Thursday, November 10, 2022
Technical Report #4	November 1 - 30, 2022	Saturday, December 10, 2022
Technical Report #5	December 1 - 31, 2022	Tuesday, January 10, 2023
Technical Report #6	January 1 - 31, 2023	Friday, February 10, 2023
Technical Report #7	February 1 - 28, 2023	Friday, March 10, 2023
Technical Report #8	March 1 - 31, 2023	Monday, April 10, 2023
Technical Report #9	April 1 - 30, 2023	Wednesday, May 10, 2023
Technical Report #10	May 1 - 31, 2023	Saturday, June 10, 2023
Technical Report #11	June 1 - 30, 2023	Monday, July 10, 2023
Technical Report #12	July 1 - 31, 2023	Thursday, August 10, 2023

DUE TO PROJECT MANAGER

Financial Status Reports (FSRs): Financial Status Reports will be submitted monthly to the AQRP Grant Manager (RoseAnna Goewey) by each institution on the project using the AQRP 22-23 FSR Template found on the AQRP website.

FSR Due Dates:

Report	Period Covered	Due Date
FSR #1	Project Start – August 31, 2020	Thursday, September 15, 2022
FSR #2	September 1 - 30 2020	Saturday, October 15, 2022
FSR #3	October 1 - 31, 2020	Tuesday, November 15, 2022
FSR #4	November 1 - 31, 2020	Thursday, December 15, 2022
FSR #5	December 1 - 31, 2020	Sunday, January 15, 2023
FSR #6	January 1 - 31, 2021	Wednesday, February 15, 2023

FSR #7	February 1 - 28, 2021	Wednesday, March 15, 2023
FSR #8	March 1 - 31, 2021	Saturday, April 15, 2023
FSR #9	April 1 - 30, 2021	Monday, May 15, 2023
FSR #10	May 1 - 31, 2021	Thursday, June 15, 2023
FSR #11	June 1 - 30, 2021	Saturday, July 15, 2023
FSR #12	July 1 - 31, 2021	Tuesday, August 15, 2023
FSR #13	August 1 - 31, 2021	Friday, September 15, 2023
FSR #14	Final FSR	Sunday, October 15, 2023

DUE TO GRANT MANAGER

Draft Final Report: A Draft Final Report will be submitted to the Project Manager and the TCEQ Liaison. It will include an Executive Summary. It will be written in third person and will follow the State of Texas accessibility requirements as set forth by the Texas State Department of Information Resources.

Draft Final Report Due Date: Tuesday, August 1, 2023

Final Report: A Final Report incorporating comments from the AQRP and TCEQ review of the Draft Final Report will be submitted to the Project Manager and the TCEQ Liaison. It will be written in third person and will follow the State of Texas accessibility requirements as set forth by the Texas State Department of Information Resources.

Final Report Due Date: Thursday, August 31, 2023

Project Data: All project data including but not limited to QA/QC measurement data, databases, modeling inputs and outputs, etc., will be submitted to the AQRP Project Manager within 30 days of project completion. The data will be submitted in a format that will allow AQRP or TCEQ or other outside parties to utilize the information

AQRP Workshop: A representative from the project will present at the AQRP Workshop in the first half of August 2023. The selected date will be updated.

Presentations and Publications/Posters: All data and other information developed under this project which is included in **published papers, symposia, presentations, press releases, websites and/or other publications** shall be submitted to the AQRP Project Manager and the TCEQ Liaison per the Publication/Publicity Guidelines included in Attachment G of the Subaward.

8.0 References

Beirle, S., Boersma, K.F., Platt, U., Lawrence, M.G., Wagner, T., 2011. Megacity Emissions and Lifetimes of Nitrogen Oxides Probed from Space. Science (80-.). 333, 1737–1739. https://doi.org/10.1126/science.1207824

Beirle, S., Borger, C., Dörner, S., Li, A., Hu, Z., Liu, F., Wang, Y., Wagner, T., 2019. Pinpointing nitrogen oxide emissions from space. Sci. Adv. 5, eaax9800. https://doi.org/10.1126/sciadv.aax9800

de Foy, B., Lu, Z., Streets, D.G., Lamsal, L.N., Duncan, B.N., 2015. Estimates of power plant NOx emissions and lifetimes from OMI NO2 satellite retrievals. Atmos. Environ. 116, 1–11. https://doi.org/10.1016/j.atmosenv.2015.05.056

de Foy, B., Saroar, M.G., Salam, A., Schauer, J.J., 2021. Distinguishing Air Pollution Due to Stagnation, Local Emissions, and Long-Range Transport Using a Generalized Additive Model to Analyze Hourly Monitoring Data. ACS Earth Sp. Chem. acsearthspacechem.1c00206. https://doi.org/10.1021/ACSEARTHSPACECHEM.1C00206

de Foy, B., Schauer, J.J., 2022. An improved understanding of NOx emissions in South Asian megacities using TROPOMI NO2 retrievals. Environ. Res. Lett. https://doi.org/10.1088/1748-9326/AC48B4

Goldberg, D., Harkey, M., Foy, B. de, Judd, L., Johnson, J., Yarwood, G., Holloway, T., 2022. Evaluating NOx emissions and their effect on O3 production in Texas using TROPOMI NO2 and HCHO [WWW Document]. ACPD. https://doi.org/10.5194/acp-2022-299

Goldberg, D.L., Anenberg, S.C., Lu, Z., Streets, D.G., Lamsal, L.N., E McDuffie, E., Smith, S.J., 2021. Urban NOx emissions around the world declined faster than anticipated between 2005 and 2019. Environ. Res. Lett. 16, 115004. https://doi.org/10.1088/1748-9326/ac2c34

Goldberg, D.L., Lu, Z., Oda, T., Lamsal, L.N., Liu, F., Griffin, D., McLinden, C.A., Krotkov, N.A., Duncan, B.N., Streets, D.G., 2019a. Exploiting OMI NO2 satellite observations to infer fossil-fuel CO2 emissions from U.S. megacities. Sci. Total Environ. 695, 133805. https://doi.org/10.1016/j.scitotenv.2019.133805

Goldberg, D.L., Lu, Z., Streets, D.G., de Foy, B., Griffin, D., McLinden, C.A., Lamsal, L.N., Krotkov, N.A., Eskes, H.J., 2019b. Enhanced Capabilities of TROPOMI NO 2 : Estimating NOx from North American Cities and Power Plants. Environ. Sci. Technol. 53, 12594–12601. https://doi.org/10.1021/acs.est.9b04488

Guenther, A.B., Jiang, X., Heald, C.L., Sakulyanontvittaya, T., Duhl, T., Emmons, L.K., Wang, X., 2012. The model of emissions of gases and aerosols from nature version 2.1 (MEGAN2.1): An extended and updated framework for modeling biogenic emissions. Geosci. Model Dev. 5, 1471–1492. https://doi.org/10.5194/gmd-5-1471-2012

Holloway, T., Harkey, M., Kim, E., Johnson, J., Yarwood, G., Goldberg, D.L., 2021. New Satellite Tools to Evaluate Emission Inventories: Is a 3-D Model Necessary? rAQRP Project 20-020.

Janz, S., Kowalewski, M.G., Lamsal, L.N., Nowlan, C., Judd, L.M., 2019. Airborne hyperspectral trace gas sensors as testbeds for geostationary air quality missions, in: Neeck, S.P., Kimura, T., Martimort, P. (Eds.), Sensors, Systems, and Next-Generation Satellites XXIII. SPIE, p. 86. https://doi.org/10.1117/12.2533765

Jin, X., Fiore, A.M., Boersma, K.F., De Smedt, I., Valin, L., 2020. Inferring changes in summertime surface ozone-NOx-VOC chemistry over U.S. urban areas from two decades of satellite and groundbased observations. Environ. Sci. Technol. acs.est.9b07785. https://doi.org/10.1021/acs.est.9b07785

Johnson, J., Wilson, G., Bandoro, J., Richman, K., Huang, L., Beardsley, R., Yarwood, G., 2018. NearReal Time Exceptional Event Modeling.

Judd, L.M., Al-Saadi, J.A., Janz, S.J., Kowalewski, M.G., Pierce, R.B., Szykman, J.J., Valin, L.C., Swap, R., Cede, A., Mueller, M., Tiefengraber, M., Abuhassan, N., Williams, D., 2019. Evaluating the impact of spatial resolution on tropospheric NO2 column comparisons within urban areas using high-resolution airborne data. Atmos. Meas. Tech 12, 6091–6111. https://doi.org/10.5194/amt-126091-2019

Judd, L.M., Al-Saadi, J.A., Szykman, J.J., Valin, L.C., Janz, S.J., Kowalewski, M.G., Eskes, H.J., Veefkind, J.P., Cede, A., Mueller, M., Gebetsberger, M., Swap, R., Pierce, R.B., Nowlan, C.R., Abad, G.G., Nehrir, A., Williams, D., 2020. Evaluating Sentinel-5P TROPOMI tropospheric NO2 column densities with airborne and Pandora spectrometers near New York City and Long Island Sound. Atmos. Meas. Tech. 13, 6113–6140. https://doi.org/10.5194/amt-13-6113-2020

Jung, J., Choi, Y., Mousavinezhad, S., Kang, D., Park, J., Pouyaei, A., Ghahremanloo, M., Momeni, M., Kim, H., 2022. Changes in the ozone chemical regime over the contiguous United States inferred by the inversion of NOx and VOC emissions using satellite observation. Atmos. Res. 270, 106076. https://doi.org/10.1016/J.ATMOSRES.2022.106076

Keller, C.A., Knowland, K.E., Duncan, B.N., Liu, J., Anderson, D.C., Das, S., Lucchesi, R.A., Lundgren, E.W., Nicely, J.M., Nielsen, E., Ott, L.E., Saunders, E., Strode, S.A., Wales, P.A., Jacob, D.J., Pawson, S., 2021. Description of the NASA GEOS Composition Forecast Modeling System GEOS-CF v1.0. J. Adv. Model. Earth Syst. e2020MS002413. https://doi.org/10.1029/2020MS002413

Koplitz, S., Simon, H., Henderson, B., Liljegren, J., Tonnesen, G., Whitehill, A., Wells, B., 2021. Changes in Ozone Chemical Sensitivity in the United States from 2007 to 2016. ACS Environ. Au 2, 206–222. https://doi.org/10.1021/ACSENVIRONAU.1C00029

Kuhlmann, G., Chan, K.L., Donner, S., Zhu, Y., Schwaerzel, M., Dörner, S., Chen, J., Hueni, A., Nguyen, D.H., Damm, A., Schütt, A., Dietrich, F., Brunner, D., Liu, C., Buchmann, B., Wagner, T., Wenig, M., 2022. Mapping the spatial distribution of NO2 with in situ and remote sensing instruments during the Munich NO2 imaging campaign. Atmos. Meas. Tech. 15, 1609–1629. https://doi.org/10.5194/AMT-15-1609-2022

McDonald, B.C., Dallmann, T.R., Martin, E.W., Harley, R.A., 2012. Long-term trends in nitrogen oxide emissions from motor vehicles at national, state, and air basin scales. J. Geophys. Res. Atmos. 117, n/a-n/a. https://doi.org/10.1029/2012JD018304

McDonald, B.C., Gentner, D.R., Goldstein, A.H., Harley, R.A., 2013. Long-Term Trends in Motor Vehicle Emissions in U.S. Urban Areas. Environ. Sci. Technol. 47, 10022–10031. https://doi.org/10.1021/es401034z

Meier, A.C., Schönhardt, A., Bösch, T., Richter, A., Seyler, A., Ruhtz, T., Constantin, D.-E., Shaiganfar, R., Wagner, T., Merlaud, A., Van Roozendael, M., Belegante, L., Nicolae, D., Georgescu, L., Burrows, J.P., 2017. High-resolution airborne imaging DOAS measurements of NO2 above Bucharest during AROMAT. Atmos. Meas. Tech. 10, 1831–1857. https://doi.org/10.5194/amt-101831-2017

Nowlan, C.R., Liu, X., Janz, S.J., Kowalewski, M.G., Chance, K. V., Follette-Cook, M.B., Fried, A., González Abad, G., Herman, J.R., Judd, L.M., Kwon, H.-A.A., Loughner, C.P., Pickering, K.E., Richter, D., Spinei, E., Walega, J., Weibring, P., Weinheimer, A.J., 2018. Nitrogen dioxide and formaldehyde measurements from the GEOstationary Coastal and Air Pollution Events (GEOCAPE) Airborne Simulator over Houston, Texas. Atmos. Meas. Tech. 11, 5941–5964. https://doi.org/10.5194/amt-11-5941-2018

Palmer, P.I., Jacob, D.J., Chance, K. V., Martin, R. V., Spurr, R.J.D., Kurosu, T.P., Bey, I., Yantosca, R., Fiore, A.M., Li, Q., 2001. Air mass factor formulation for spectroscopic measurements from satellites: Application to formaldehyde retrievals from the Global Ozone Monitoring Experiment. J. Geophys. Res. Atmos. 106, 14539–14550. https://doi.org/10.1029/2000JD900772

Platt, U., Stutz, J., 2008. Differential Optical Absorption Spectroscopy. Differ. Opt. Absorpt. Spectrosc. https://doi.org/10.1007/978-3-540-75776-4

Souri, A.H., Choi, Y., Pan, S., Curci, G., Nowlan, C.R., Janz, S.J., Kowalewski, M.G., Liu, J., Herman, J.R., Weinheimer, A.J., 2018. First Top-Down Estimates of Anthropogenic NOx Emissions Using High-Resolution Airborne Remote Sensing Observations. J. Geophys. Res. Atmos. 123, 3269–3284. https://doi.org/10.1002/2017JD028009

Zawacki, M., Baker, K.R., Phillips, S., Davidson, K., Wolfe, P., 2018. Mobile source contributions to ambient ozone and particulate matter in 2025. Atmos. Environ. 188, 129–141. https://doi.org/10.1016/j.atmosenv.2018.04.057